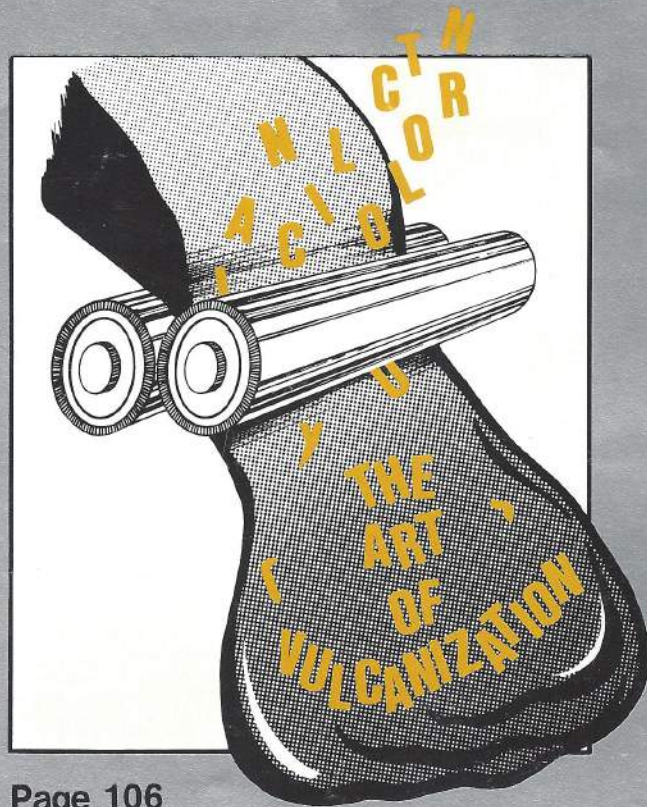


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Modeling: The rules of the game

"We are like the sailors who must rebuild their ship on the open sea, never able to dismantle it in drydock and reconstruct it there out of the best materials. . ."

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Today's criteria of project success include not only simple profit calculations, but an assessment of the effects of inflation and the risks of unexpected changes in markets, feedstocks, and environmental and trade regulations. Technologists cannot ignore these external parameters, for the only workable engineering models are embedded in a matrix of models of economics, ecology, politics, organizations, societies, and the world economy.

This article outlines a strategy of modeling that's based on an examination of the philosophy of modeling. First, we'll discuss the nature of modeling, why we build models, and the difficulties and limitations of models. Then we'll discuss a model of how technical models are embedded in social science models.

A model is . . .

The term "model" is often used loosely to refer to any scientific theory couched in symbolic, postulational, or formal styles. A large literature discusses the relationships among models, theories, analogies, and metaphors. We can summarize it as follows.

Cognitive styles differ by gradations in the degree of mathematization. First is the *literary*, or narrative style, in which a plot is unfolded, and a particular sequence of events is described. The history of a technical development (e.g., the discovery of antiknock compounds), or a report of progress on a particular project (e.g., construction of a pilot plant, as in Kohl et al. (1)) are in this category. Second is the *academic* style, in which an abstract, general discussion is presented. There is an attempt to be precise, but it is verbal and a special technical vocabulary might be used (e.g., a review of the state of the art in flash hydrolysis). A third style is *eristic*, or argumentative. There is a strong interest in proof, and in specific propositions, rather than in exhibiting possibilities in broad perspective. Experimental and statistical data become important. Attention is given to deductive relationships and logical derivations from propositions previously established, or explicitly assumed, though proofs are sketched rather than rigorously laid out. There is considerable awareness of the scientific method. An example of this style would be a discussion of indirect liquefaction of coal and its advantages and disadvantages compared to direct liquefaction (2).

Fourth is the *symbolic* style, in which mathematics comes into its own. The subject is conceptualized from the outset in mathematical terms. In this style, computers are likely to play a major role (one example is a discussion of a new algorithm for distillation design) (3). The fifth style is *postulational*. Here, the validity of proof is the focus of attention, rather than content of the propositions. Rules for derivations are explicitly formulated and applied. The foundation on which the whole system is erected is a set of propositions laid down to serve in just this way. These are the postulates. From them, theorems are derived whose

verification indirectly validates the postulates by which they are proved. Interest centers on the independence of the postulates from one another, and on their mutual consistency. What is wanted is the simplest set that will suffice for the derivation of the theorems in which we are interested (e.g., derivation of the basic laws of thermodynamics) (4). The sixth style, the *formal* style, is close to the *postulational* style, and indeed presupposes it. The difference is that here the key terms are not given any interpretation; there is no reference to any specific empirical content. In general, a number of different interpretations can be given to the formal system, with equal justification, insofar as the system itself is concerned. The formal style is "pure" mathematics (an example is the general solution for quadratic equations).

Why model?

Among the uses of models are organizing data and communicating ideas (5), lending clarification, and permitting the handling and extrapolation of complex relationships. Furthermore, models can reveal gaps and remove ambiguity. The principal reason for modeling in the practical world of technology is economically to manipulate complex systems of ideas, in order to predict what will happen in the real world. One kind of model may be used to design a system, another to design its components, etc.

The problems of modeling

One problem shared with all modeling techniques is the tendency to overemphasize method over content. The "Law of the Instrument" tells us that if you give a child a hammer, he will find that everything needs hammering. Thus follows ". . . the conviction that what the scientist is able to do and would like to do is called for by the scientific situation or by the nature of science itself" (5). An example in the fossil energy field is the frequent appearance of kinetic studies of coal gasification reactions, reflecting widespread knowledge of kinetics, while no attention is paid to the problems of real gasifiers—controlling the formation of ash clinkers, for example.

Another problem that afflicts model builders is overemphasis on symbols. We identify this tendency with the unconscious belief in the magic of symbols, which runs through history from Pythagoras through the Cabbalah to Kepler and in our journals and a well-known text on transport phenomena (6).

Still another problem is overemphasis on form, that is, identifying truth with a logical system and order so that the model itself becomes the object of interest, and thereby limits our awareness of the unexplored possibilities of the subject matter. The literature on optimal control theory and optimal temperature profiles for one-dimensional plug-flow reactors are examples of this hang-up.

Then there is oversimplification. A model is inevitably

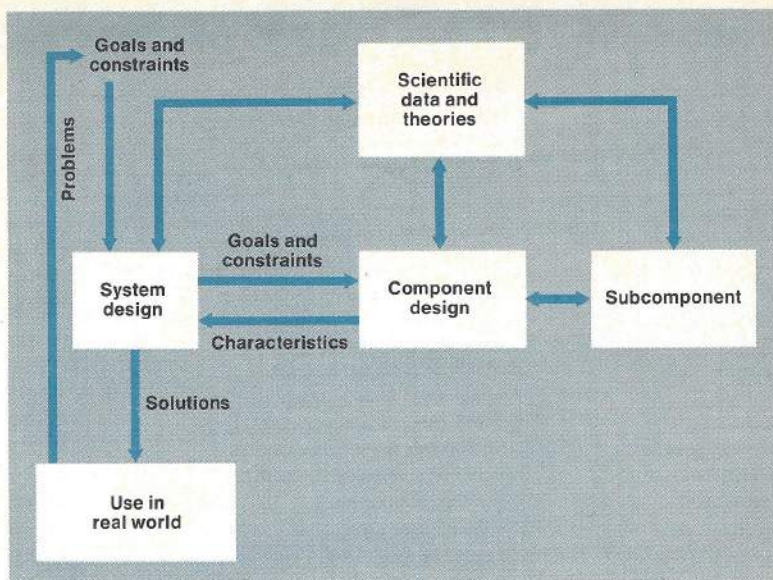


Figure 1. Model of engineering

simpler than the subject matter, yet a great deal depends on how and why the simplification was made. It is one thing to neglect a feature that is not essential, at least to the degree of accuracy being sought. It is quite another to follow the principle of the "drunkard's search":

A drunkard was searching under a streetlight for his housekey, which he had dropped some distance away. When asked why he didn't look where he dropped it, he replied, "The light is better here."

Models based—unconsciously, of course—on this principle are simple, elegant, and so much easier to work with. An example in the fossil fuels processing field (where there are many) is the use of a continuous stirred-tank reactor model to represent a fluidized-bed coal gasifier. In such a gasifier the important problems are related to temperature variations, and the economics depends on the steam consumption required to control the temperature variations. Yet in the continuous stirred-tank reactor, there are no temperature variations, because it is "well-stirred" by definition.

Another failing of model builders consists of an undue emphasis on exactness and rigor (a subject we'll explore later).

"Map reading" is another pitfall. It is the danger that all features of the model will be assumed to correspond to characteristics of the subject matter. For example, one might conclude that Greenland is bigger than Australia, because that is how it looks on the map. Similarly, some have mistaken the geometric arrangement in a process flow diagram for an actual equipment layout. A related error is "pictorial realism." The map reading error consists of a failure to distinguish properly between the essential and the irrelevant properties of the model, and treating as relevant properties that are irrelevant. We must not lose sight of the fact that the model gives a limited perspective. It may exhibit characteristics that are not important from another perspective, and omit characteristics that from another perspective are important. We may misconceive a model as an image or likeness of what is being modeled. The mistake of pictorial realism is in forgetting that the similarity exists only in a given perspective. An analogy has been made with the Third Commandment, "Thou shalt not make unto

thee any graven image." An image is constituted neither by its form nor by its substance, but by the idolatry of its worshipers (example: classical economics and the neoclassical revisions).

Requirements for a good model

Von Neuman and Morgenstern (7) have taught us that

... the definition must be precise and exhaustive in order to make mathematical treatment possible. The construct must not be unduly complicated so that the mathematical treatment can be brought beyond the mere formalism to the point where it yields complete, numerical results. Similarity to reality is needed to make the operation significant. And this similarity must usually be restricted to a few traits deemed "essential" *pro tempore*—since otherwise the above requirements would conflict with each other.

The only thing that will completely represent in every respect and in all the details something as complex as an airplane, a cat's brain, or a chemical process, is the thing itself. But no purpose is served in reproducing the prototype. Models are simplifications of the real world in which you select the kind and amount of detail the model ought to incorporate to do its job.

The need to produce numerical results forces models to stay within the limits of computability. Our ability to comprehend complex systems is also a limitation. We lose confidence in very complex systems, regardless of formal "proofs." Experience with "proofs" that turn out to be fallacious convinces us that a complex model is more likely to be incorrect. Developing confidence in a model is a social process.

If we do not wish to use the real thing or models as complex as they are, how do we go about simplifying systems for modeling? The question that usually leads to means for simplifying the system is "Why model?" If we want a model of a chemical plant that shows spatial relationships and the appearance of the plant, it can be constructed out of wood and plastic and will have certain similarities to the prototype. If we want a model that shows the sequence of processing steps and the flow of material and energy, we will construct a process flow diagram. The kinds of details that are represented and those that are omitted are dictated by the kind of questions that will be asked of the model. Engineers

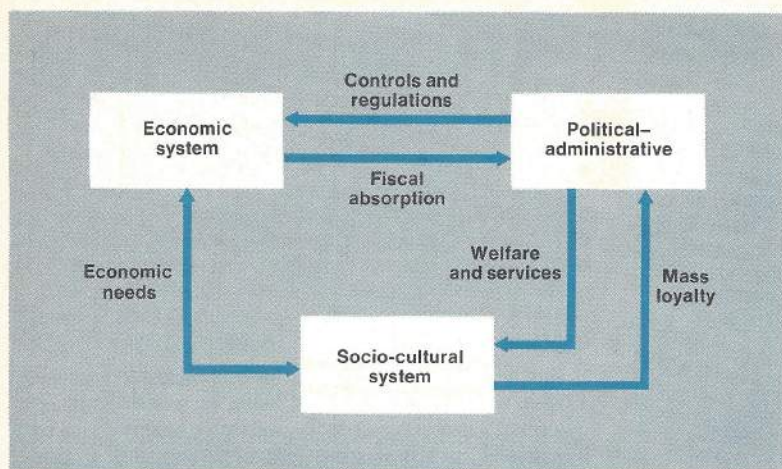


Figure 2. Social organization

are more fortunate than scientists, since their goals are usually laid out before them. Whereas the scientist is supposed to find truth, the engineer must only solve practical problems. Even if he finds a solution without finding understanding, he is considered to be successful.

Models of science and engineering themselves

The bulk of the literature on the philosophy of science contains an idealized model of science. In this model, we have two realms: the realm of fact and the realm of theory. There is a clear distinction between the object being observed and the observer. It is presumed that by some discovery process (which is outside the purview of the scientific method) a set of postulates has been laid down, from which, by logical operations, a theory is deduced. The theory makes predictions about the real world. These predictions depend on the "truth" of the postulates, and on the correctness of the logic used. *No amount of verification of a theory will prove it true.* However, if a prediction of the theory is proven false by *facts*, the theory is proven untrue. The next step is to determine where the error lies. If the logic is not faulty, the postulates may have to be changed, perhaps drastically, and a completely new theory may result. That is the way it has worked out, at least in some areas of theoretical physics such as mechanics and electromagnetic theory. But we know that when we make a measurement that contradicts the Second Law of Thermodynamics, we immediately question the measurement. Everyone who has done experiments knows about unexplained anomalies in data. Why is it that sometimes we have more faith in the theory than in the observations—the facts?

An alternative and more modern view of science helps to put all this into perspective (8). This view holds that scientific knowledge must be viewed as a coherent network, in which some of the strands are theoretical and some are observational. This construct supports our overall confidence even when elements of the network are found to be incorrect. Since almost all observations are made with the use of instruments, and in the light of theories, these observations are "theory laden." Therefore, as in the older model, one practically never confronts a purely theoretical

statement with a purely observational statement (fact). One merely confronts deductions from one set of theoretical propositions with the conclusions from another set. When there is an inconsistency, the question then becomes "Which theory is likely to be falsified?" When a data point falls far from the curve, the experimenter will question the assumptions that put that data point in the same population as the others. He may conclude, for example, that the point belongs in another population because water pressure changed erratically when "someone must have flushed a toilet." The network model of scientific theory is thus consistent with the social processes of the scientific community.

If science is a social product, engineering must be more so. Figure 1 shows our model of engineering. The goals and constraints for technology are set externally. The technologist is supposed to devise the systems and schemes for satisfying those goals, under the imposed constraints, using the data and theories of science. Sometimes, as in a business enterprise, the purpose of the engineering project is to make a profit, but the constraints, i.e., the availability and cost of capital, and the accounting rules, come from the social system. Sometimes the goal is not profit, but satisfaction of an environmental constraint, a purpose rooted in "national defense," "national pride," overcoming institutional barriers, or a variety of other purposes that are not easily expressed in economic terms. In recent years, our Apollo space program and the comparable Soviet program were motivated by considerations of national pride and intellectual curiosity. At times, individuals and organizations engaged in the programs were motivated by strictly economic goals, which were artificially created to use a market economy to achieve noneconomic goals. The government's intervention in the economy is usually justified by a desire to achieve goals that might otherwise not be attainable. An example is support of scientific research, which while likely to benefit all, cannot be expected to benefit a single company enough to support the work. More obvious examples are police and fire protection, and highway and port operation. Since it is often difficult to frame the goals in market economy terms, and sometimes the market model gives an answer we feel intuitively is

Computational limits

It is surprisingly easy to set up a computational problem that goes beyond the limit of computability. But without calling on the limits of computability, one can usually estimate the computational requirements of a model and determine whether it can be considered practical. For example, if a certain model requires operations computationally equivalent to enumerating the permutations of a deck of cards, can we consider this computable? The number of possibilities is 52 factorial, or about 8.07×10^{67} . If we assume that one permutation per nanosecond is pretty speedy, that gives us a minimum requirement of 2.56×10^{51} years of computer time. Should someone point out that parallel computations were the answer, we can re-scope the problem by putting everyone on earth to work with a one-permutation-per-nanosecond computer. Assuming 4×10^9 people, that reduces the time to . . . Need we continue?

wrong, one social science model that should be questioned is the market model in economics.

Take the specific case of synthetic fuels. We feel that tax and accounting practices have been responsible for the failure of such projects to be economically competitive (9). However, it has become clear that an intervention in the market system is necessary to make synthetic fuels "economic" (whatever that means), either to correct distortions in the market caused by other government interventions or to deliberately distort the market to satisfy some other needs, such as political independence, or merely national pride.

Models in social sciences

In the social sciences, there is a fundamental limitation on any effort to develop causal models, because the system incorporates human behavior. Human beings are the only objects of analysis that are capable of reading the analysis and of anticipating the logic of a causal model. They may and often do act in ways that make the analysis false.

To illustrate, we will call attention to three areas in which social science models are important to engineers: the model of economics and society, the model for decision-making processes, and models of organizations.

On economics

To conceptualize the organization of society (10), three organizational principles are identified (Figure 2):

- economic
- political-administrative
- socio-cultural.

They are based, respectively, on exchange, coercion, and normative structures.

If we visualize the economic area as dominant, and reduce regulatory inputs and fiscal drain of the political area, we see roughly the "early capitalism" described by Adam Smith and Karl Marx. For various reasons, modern industrial societies have deviated from this picture in the way indicated in the diagram. The result has been that (11):

Neither the economist nor anyone else has developed the conceptual frame required to comprehend and to deal rationally with group behavior and collective choice in a multisectoral economy, where planning and programming in the political

economy and participatory planning in the market economy have, by force of circumstances, become a commonplace necessity. But, if all alike share the blight of ignorance, the economist additionally bears the burden of his knowledge. His cognitive framework positively excludes and rules out of account a priori those functions and values that are now at the heart of economic organization and control in all advanced industrial societies.

Furthermore, "Wherever an anthropologist looks, he sees a tribe; wherever a sociologist looks, he sees a family; and wherever an economist looks, he sees a business run by a hardnosed profit-seeking entrepreneur in a price-competitive market" (11).

On decision making

Often in models of economic theory and in management science a basic assumption is made that consensus can be reached on goals, on the means of reaching the goals, and on how to evaluate the solutions. It is implicit that this consensus is understood by all concerned, so that optimum solutions can be found by calculation. However, when there are diverse groups, with varying goals, interests, and perceptions, they may or may not agree on goals, means, or even on the model of the world in which the problem exists.

Comprehension limits

Himmelblau's law states that 25% of all analytical partial derivatives are incorrect. Breed's law says that 75% of all corrections are errors. And Stanley Katz is reputed to have asked a student, "Do you really believe that, or did you only prove it?"

In Figure 3 we analyze a situation in which two groups are involved, leading to four possibilities. In the upper left box, the decision is made by calculation (the management science situation). This only means that both groups agree on how to decide, not that anyone is right. When goals are not shared, but the understanding of the problem is shared, the way is open to bargaining (I'll give up something if you give up something else). When goals are shared, but there is a disagreement on strategy, the decision takes the form of judgment, i.e., some kind of impartial evaluation of strategies in an attempt to satisfy everyone. Inspirational or charismatic decision making is the last resort, when nothing else will work. This model serves to show why an "optimal" solution technique doesn't always help.

On organizations

Benson et al. (12) comment that various theories of organization are based on assessment of functions and dysfunctions from a certain point of view, but leave the development of that viewpoint unexamined. What happens when a new organization is created from an old one? The

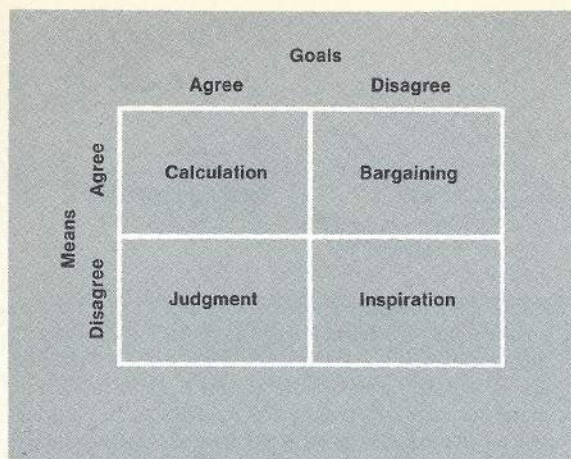


Figure 3. Decision making

motives for reorganization usually come from a drive for purely administrative goals, i.e., efficiency, rational budgeting, control, and planning. For these goals we get, as solutions, centralization and decentralization, as well as different principles of organization. It could be by raw material source, or by market, or by production technology, or by professional discipline, and sometimes by more than one, as in matrix management. In the Energy Research and Development Administration it was by type of energy source. Another choice is to cut across the lines of energy source and group functions by degree of advancement, i.e. basic research, development, commercialization, and production. That is how DOE was set up. We call the process "vortex management."

Underneath it all is the assumption that the two-dimensional graphs, which we call organization charts, are a *model* for the human activity. What is overlooked in setting it up is that the administrative goals, "efficiency, rational budgeting, control, and planning," lack a core—that is, a clear-cut mission or purpose for the organization. The program-oriented people in the organization usually are committed to substantive goals, and will defend the old arrangements. The conflict comes from a desire to fulfill their program, keep their turf, and maintain their resources. The professional people derive their power from their technical expertise, external constituencies, and the ability to leave for the outside labor market.

Thus, in the real world organizations are not as simple as they seem in the model—the two-dimensional graph. We have a multiplicity of goals, limited resources, and inherent conflict between professional administrators and program-oriented professionals. Whatever the organization chart shows, if you have general agreement on the organization's goals, and don't reorganize so often that no one knows where anything is, motivated individuals will find the informal routes for getting the job done.

Conclusion

In technology many of the most important models are not models in the physical sciences or of systems and components. Social, political, and economic factors (if these can be divided into separate areas) determine the goals, resources available, constraints, ground rules, and even how we organize ourselves to do the work. If we want to make technology a more rational activity and improve on intuitive

practices, we believe that these are the areas most in need of critical scrutiny by technologists in particular, because they work at the intersection of science and society. And they need to "... rebuild their ship on the open sea ..." (13).

References

- (1) Kohl, A. L.; Harty, R. B.; Johanson, J. G.; Naphtali, L. M. *Chem. Eng. Prog.* 1978, 74(8), 73-79.
- (2) Shinnar, R. *CHEMTECH* 1978, April, 686-693.
- (3) Naphtali, L. M.; Sandholm, D. P. *AIChE J.* 1971, 17, 148-153.
- (4) Naphtali, L. M. *AIChE J.* 1960, 12, 195-197.
- (5) Kaplan, A. "The Conduct of Inquiry"; Chandler: New York, 1964.
- (6) Bird, R. B.; Stewart, W. E.; Lightfoot, E. N. "Transport Phenomena"; John Wiley & Sons, Inc.: New York, 1960.
- (7) von Neumann, J.; Morgenstern, O. "Theory of Games and Economic Behavior"; John Wiley & Sons, Inc.: New York, 1964.
- (8) Hesse, M. "The Structure of Scientific Inference"; University of California Press: Berkeley, Calif., 1974.
- (9) Naphtali, L. M.; Shinnar, R. *Chem. Eng. Prog.* 1981, 77(2), 65-71.
- (10) Offe, C. *Int. J. Politics* 1976, Fall, 29-67.
- (11) Solo, R. A. In "Stress and Contradiction in Modern Capitalism"; Lindberg, L. N. et al., Eds.; Lexington Books, D.C. Heath & Co.: Lexington, Mass., 1975.
- (12) Benson, J. K.; Cook, J.; Riddle, R. "Contradiction and Organizational Change: Reorganization in a Natural Resources Department"; presented at the 9th World Congress of Sociology, Uppsala, Sweden, August 1978.
- (13) Neurath, O. "Logical Positivism"; The Free Press: Glencoe, Ill., 1959.

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